# Design and Performance of a Compact Collimator on GM/CA-CAT At the Advanced Photon Source

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## ABSTRACT

A new macromolecular crystallographic facility developed by The General Medicine and Cancer Institutes Collaborative Access Team (GM/CA-CAT) at the Advanced Photon Source (APS) is a part of the Biosciences Division (BIO), Argonne National Laboratory (ANL). The facility consists of three beamlines: two lines based on the first "hard" dual canted undulators and one bending magnet beamline [1]. Several compact collimator systems have been developed for the purpose of background reduction in macromolecular crystallography experiments. The apparatus consists of a tube collimator, pinhole and kinematics mount. This paper will present a series of compact collimator designs and crystallographic applications based on experimental requirements [2]. We also describe the magnet-based kinematic mounting structures [3] developed as a collimator holder.

Keywords: mini-collimator, kinematic mount, crystallography

## 1. INTRODUCTION

The Advanced Photon Source (APS) at Argonne National Laboratory (ANL) is a national user facility for synchrotron radiation research. A new macromolecular crystallographic facility developed by GM/CA-CAT is operational at the Advanced Photon Source (APS). The facility consists of three beamlines: two lines based on the first "hard" dual canted undulators and one bending magnet beamline. The GM/CA CAT canted undulator beamlines at the APS already provide high intensity focused beams of approximately 20 x 70 microns at the sample position. The samples are held on a high precision air-bearing based goniometry. This case is called "normal beam". To meet the growing user needs of smaller sample crystals, a "mini-beam" apparatus has been developed which conditions the beam to about 7 microns (FWHM) diameter. We refer to this as the "mini-beam" set-up. Several compact collimator systems are in use for macromolecular crystallography. The primary advantages are beam definition and background reduction.

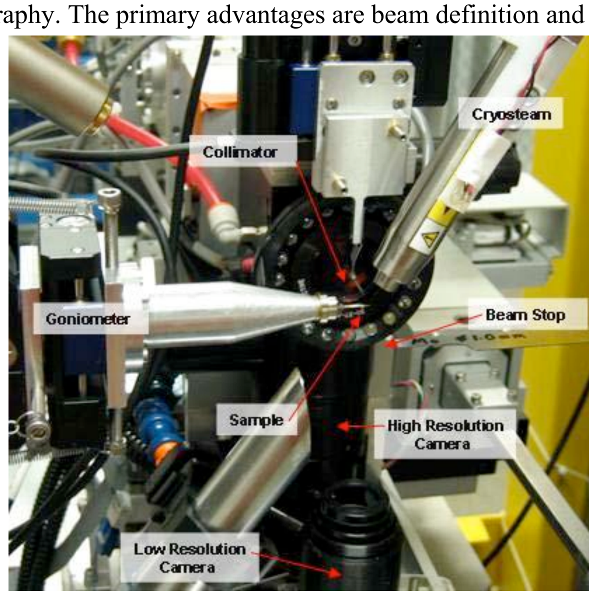


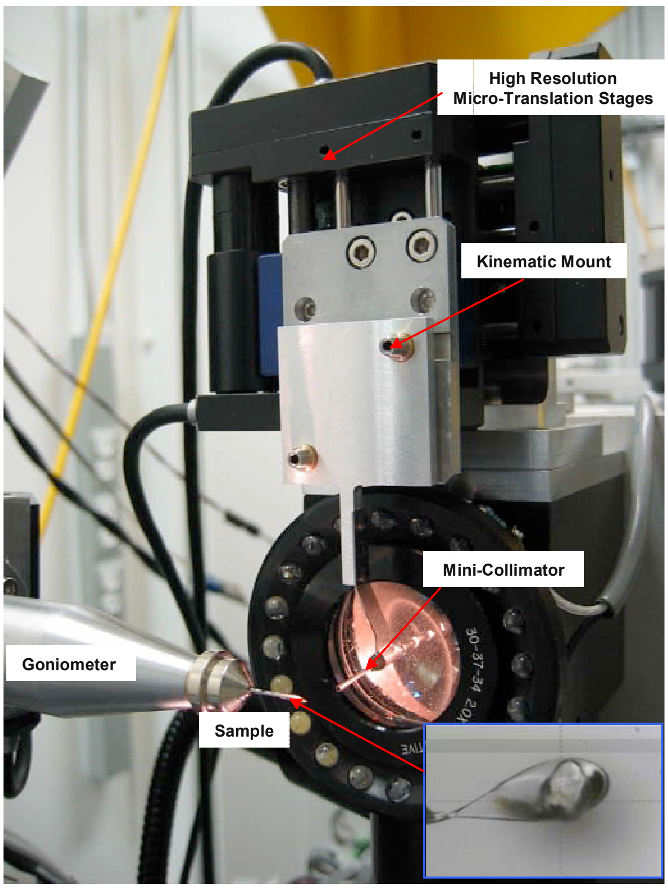

Figure 1. Overview of the GM/CA experimental stations.

New Developments in Optomechanics, edited by Alson E. Hatheway,
Proc. of SPIE Vol. 6665, 66650X, (2007)
0277-786X/07/$18 · doi: 10.1117/12.733173

The collimating system consists of tube collimator, pinhole and kinematic mount. This paper will present a series of compact collimators designed for use in macromolecular x-ray crystallography. This new design employs a magnetic base kinematic mounting system developed for holding the collimator assembly vertically.
The instrumentation and sample environment set up can be seen in Fig.1.

## 2. COLLIMATOR DESIGN

The compact collimator is located near the focal position and employs 5, 10, 100, 300 or 600 micron pinholes coupled with a tungsten or molybdenum scatter guard with a very small diameter tube serving as a forward scatter guard. See Fig. 2. The apparatus has a kinematic mount that allows easy exchange between the normal beam collimator (300 μ or 600 μ pinhole) and mini-beam collimator (5 or 10 μ pinhole).



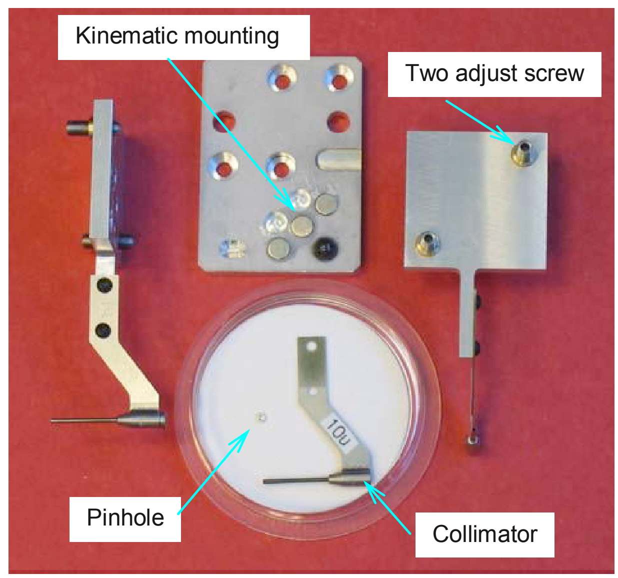




Figure 2. Close up of the collimating system on the OAV (left picture), the collimator consists of a tube collimator, pinhole and kinematic mounting system (right side picture)

### 2.1. Mechanical design of the collimator system

The components and its implementation can be seen in Fig. 2. The detailed technical data is shown in the Tables 1-3 below. The collimating system follows the OAV (On-Axis Visualization) system. The On-Axis-Visualization system provides a parallax-free image of the direct beam at the sample position. This is accomplished by mounting a front-surface mirror at an angle of 45 degrees to reflect the image of the beam from a YAG scintillator at the sample position down to a 16:1 zoom optics and digital color CCD camera. Both the mirror and the objective lens nearest the sample have a 1.2 mm hole to allow passage of the x-ray beam. The on-beam-axis video microscope and YAG crystal are used to visually align the beam to the sample position. The collimator apparatus is located between the lens and the sample. It employs a pinhole coupled with scatter guards. A high degree of beam positional and intensity stability is achieved, in part, because the focused beam overfills the aperture.

Two PI-M-111 high resolution micro translation stages are combined to form a xz system for the collimator alignment. A kinematic mounting system is designed for collimator vertical mounting. In Fig.2, the top center picture shows the kinematic system consisting of one 4.76mm diameter ceramic ball, three pairs of rare earth magnets, and two precision adjustment screws. The ceramic ball and magnets ensure smooth and reliable motion. The two precision screw sets are installed on the holder plate. These screws feature tight tolerance and no excess grease. The gap between the two plates is 1 mm. The distance from screw to control ball is 20 mm. The kinematics mounting set has a range of ± 2.7° for tilt using the adjustment screws, brass nuts and the ball.

Kinematic mounting principles are extensively applied to the mechanical structure design for high-precision instruments. The kinematic design is deterministic and does not rely on a probabilistic approach. Kinematic mounting can provide repeatable relocation capability with high accuracy, which is very important for many synchrotron radiation experimental applications, such as the compact collimator for x-ray crystallography.

The kinematic mount for this collimator allows quick change of different aperture diameters (5, 10, 300 and 600 microns) according to sample size.

The tube collimator serveing as a beam shield is inserted into the hole of a tapered cylindrical holder, see Fig. 3.

## 2.2. Technical data of collimator

### 2.2.1. High resolution stages

The two PI-M-111 high resolution micro translation stages are combined to form the XZ system for the collimator horizontal and vertical alignment. The X direction is horizontal, perpendicular to the X-ray beam. The Z direction is vertical, perpendicular to the X-ray beam**.**

**TABLE 1: High resolution PI M-111.1DG stage specifications**

| | |
|---|---|
| Travel Range | 15 mm |
| Design resolution | 0.007 µm |
| Unidirectional repeatability | 0.1 µm |
| Max. normal load capacity | 3 kg |

### 2.2.2. Kinematic mount

**TABLE 2: Kinematic mounting parts**

| | |
|---|---|
| **Magnet neodymium iron boron** | |
| Shape | Disc |
| Diameter | 0.1875" [4.76 mm] |
| Thickness | 0.0625" [1.58 mm] |
| Material | NdFeB 42 |
| Gauss | 1.25 lbs lift |
| **Precision #6-80 screw for pitch adjustment** | |
| Tip Style | Ball |
| Threads per inch | 80 |
| Travel | 0.08" [2.0 mm] |
| Screw Length | 0.43" [11.4 mm] |
| Resolution/11.25° Turn in holder | o.5 mrad |
| Resolution/5° Turn in holder | 0.222 mrad |
| **Positioning Ball** | Ø4.76 ceramic ball |

The most common type of kinematic mount is the cone, groove, and flat mount illustrated in Figure 2. Consider the collimator as being attached to the coordinate system of the one ball and two adjusting screw in the figure 2 and its corresponding mount having the cone, vee, and flat. For the new design, the 4.76 mm diameter ball is first glued in the cone. The screw with a sphere end is seated in the groove, which is aligned towards the cone. This constrains or eliminates two more degrees of freedom, pitch and yaw, as shown in the Figure 2. The alignment of the groove towards the cone is important in order not to over-constrain one or more of the translation degrees of freedom. Finally, there is only one degree of freedom left to constrain, roll about the Y-axis. This is accomplished by seating the third sphere of the screw on the flat. The advantages of a kinematic mount is increased stability, three pairs of rare earth magnets exerts more than 6 lbs of force to hold the collimator.
The NEWPORT adjustment screws have precision rolled threads for exceptionally smooth adjustment and higher sensitivity than standard micrometers.

### **2.2.3.** Beam defining aperture and beam shielding capillary

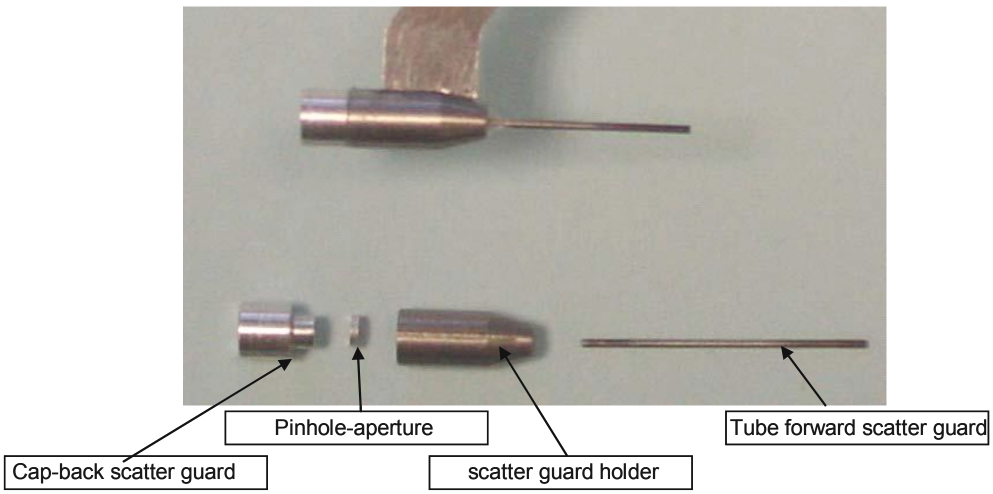



Figure 3. Close up of the collimating

**TABLE 3: Scatter guards and apertures of collimator**

| | |
|---|---|
| **Cleaning aperture-pinhole** | |
| Pinhole Material | Platinum-Iridium 2mm O.D. X 0.6mm Thickness |
| Pinhole Size | 5µ, 10µ, 100µ, 300µ and 600µ |
| **Beam shielding holder** | |
| Holder (scatter guard) Material | Molybdenum |
| Holder (scatter guard) Dimensions | Ø3.5 mm X 9 mm length taper cylinder |
| **Beam shielding Tube** | |
| Tube (forward scatter guard) Material | Molybdenum |
| Tube (forward scatter guard) Dimensions | Ø0.79 mm I.D, Ø1.05 mm O.D for 600µ pinhole for BM commissioning |
| | Ø0.79 mm I.D, Ø1.05 mm O.D for 300µ pinhole for BM regular |
| | Ø0.79 mm I.D, Ø1.05 mm O.D for 300µ pinhole for ID regular |
| Tube (forward scatter guard) Material | Tungsten |
| Tube (forward scatter guard) Dimensions | Ø0.40mm I.D, Ø1.0 mm O.D for 10µ pinhole for ID mini beam |
| | Ø0.40mm I.D, Ø1.0 mm O.D for 5µ pinhole for ID mini beam |
| **Cap-back scatter guard** | Ø3.5 mm X 9 mm length cylinder |

Figure 4. Several interchangeable collimators with size pinhole as 5μ, 10μ, 100μ and 300μ have been assembled for experimental needs. The 5μ and 10μ pinhole used for Mini beam and 300μ pinhole used for normal beam applications.

### 2.3. Device for pre-alignment of all collimator

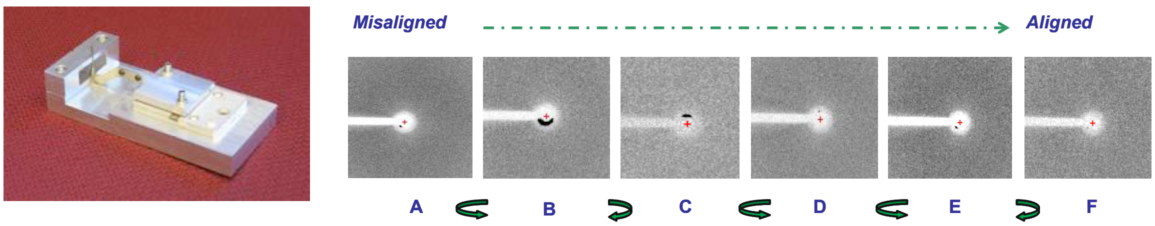



Figure 5. A device for pre-alignment was designed. See left picture. After pre-alignment the collimator can be aligned in 15 minutes

The Device for pre-alignment was designed. It is specifically built for the GMCA compact collimator device alignment. It enables the precise positioning of the shielding guard to the collimator tube. The sequence of pictures to the right in Fig.5 shows images of interference patterns produced from x-rays clipping the pinhole. The images are recorded downstream on the MAR300 CCD detector. The dark spot in the center is due to the misalignment of the collimator tubing. Using the two adjustment screws the collimator yaw and pitch can be aligned. Image A was the first image, then the vertical adjustment screw was turned a 1/4 CW (Image B). Then the vertical adjustment screw was turned 1/8 CCW (Image C), then the vertical adjustment screw was turned 1/16 CW (Image D), then the vertical adjustment screw was turned 1/32 CW (Image E), finally the vertical adjustment screw was turned 1/32 CCW (Image F), DONE!! the 10μm collimator is straight.

## 3. measurements results

### 3.1. Results of repeatability of the kinematic mounting

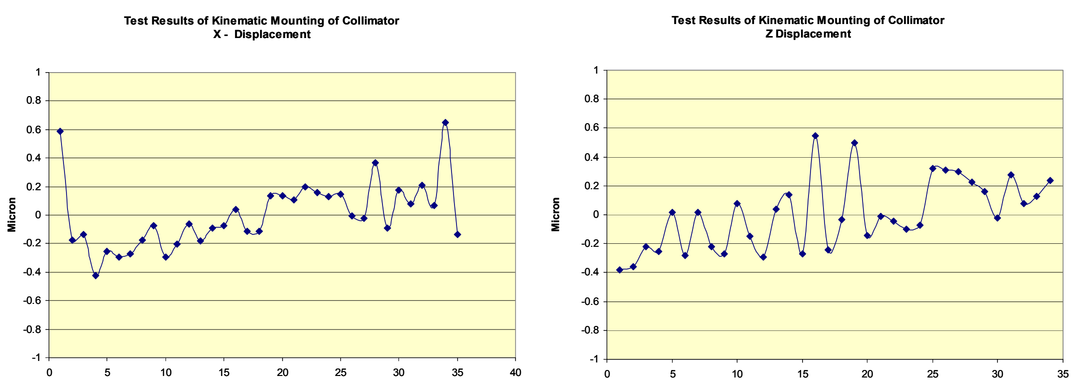



Figure 6. The test results of repeatability of kinematic mounting is within ± 0.4 μ

### 3.2. Results of stability of the kinematic mounting

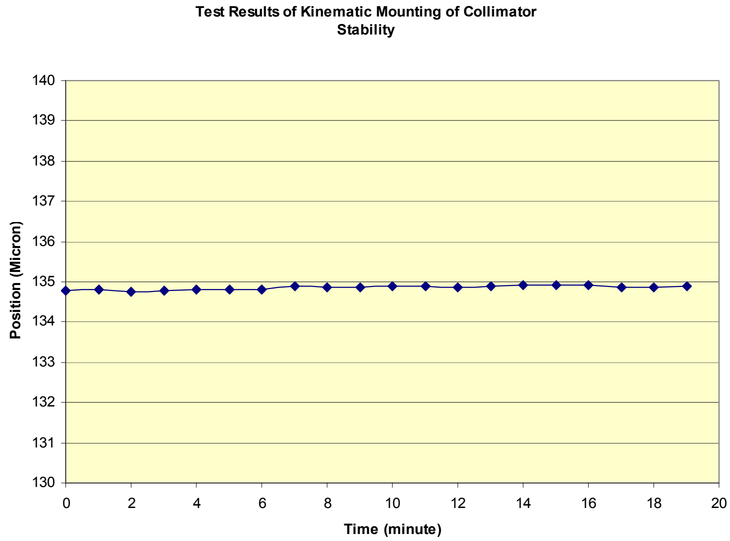



Figure 7. The test results of stability of the kinematic mounting is within ±0.1μ

We used the Keyence scanning laser confocal displacement meter set in in-profile mode to perform repeatability and stability tests for the compact collimator mounting system.

The test results of the mechanical repeatability of the kinematic mounting apparatus of the collimator show both horizontal and vertical displacements in the ±0.4μ range (Fig. 6) the result of the stability test shows the position was stable, with the displacements in the ±0.08μ range (Fig. 7) over twenty minutes.

## 4. APPLICATION AND DEVELOPMENT

### 4.1. "Mini beam"

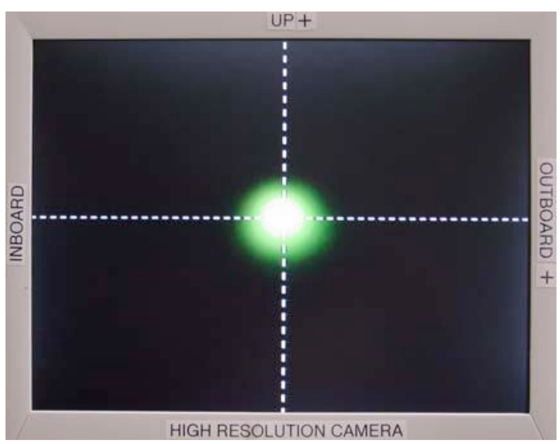



Figure 8. Mini-beam imaged on the YAG crystal mounted at the sample position.

GM/CA CAT developed a "mini-beam" apparatus that conditions the beam to about 5 microns (FWHM) diameter with an intensity of ~$7 \times 10^{10}$ photons/sec when the pinhole diameter is 5 microns. The beam is approximately 7 microns (FWHM) diameter with an intensity of ~$1 \times 10^{11}$ photons/sec for the 10 micron pinhole.

### 4.2. Future development of the mini-beam

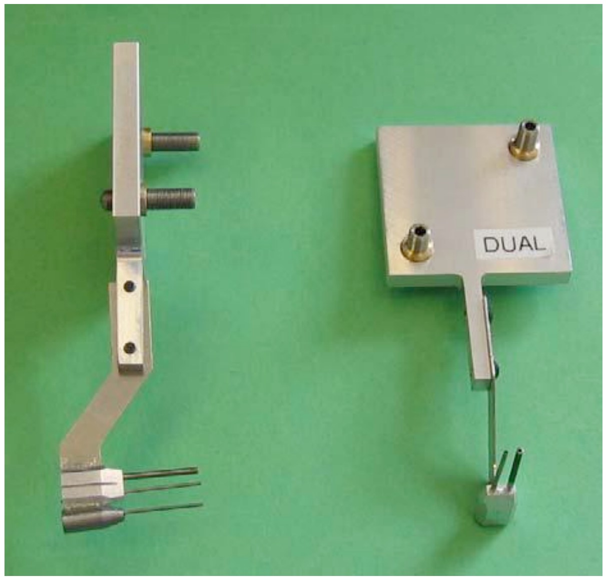



Figure 9. The Double and triple collimator was developed in study

Double and triple collimators, Figure 9, have been developed for further study. We will need to solve the alignment challenge prior to its use. Double collimators can be used for optimal data collection from large crystals as well. For example, the sample can be probed with the mini-beam first to find the best regions and then data collected with the larger beam. Triple collimator can be used to better fit beam to the sample size.

## 5. SUMMARY

The compact apparatus is achieved:
1. Scatter guards reduce background significantly.
2. Mini-beam apparatus: small beam-defining pinholes.
3. Precision quick-change
4. High repeatability and stability
5. After pre-alignment easy and quick to align
6. Can be adapted to other beamlines

## 6. ACKNOWLEDGEMENT

**GM/CA CAT has been funded in whole or in part with Federal funds from the National Cancer Institute (Y1-CO-1020) and the National Institute of General Medical Science (Y1-GM-1104).
Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Basic Energy Sciences, Office of Science, under contract No. DE-AC02-06CH11357.

We thank D. Yoder, R. Sanishvili, V. Nagarajan, M. Becker, S. Corcoran and J. L. Smith for helpful discussion and support.

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